Can We Predict Contact Angle with Molecular Dynamics Method?

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Liquid-solid contact or wetting is very important for the phase change heat transfer such as boiling and condensation. The molecular scale understandings of 'contact angle', '3 phase contact line', or 'liquid precursor film' are desired for the proper modeling of wetting phenomena [1]. We have simulated the equilibrium liquid droplet [2], vapor bubble nucleation [3], and liquid droplet nucleation [4] on the solid surface for the simple Lennard-Jones fluid system; by artificially changing the potential parameter between fluid and solid molecules, considerable information is obtained about the wetting of surface. Now, we challenge the prediction of contact angle by the molecular dynamics method for realistic combination of fluid and solid, water on platinum surface [5, 6].

Water molecules were modeled with the SPC/E model [7] and the platinum surface was represented by three layers of harmonic molecules. The phantom molecules were used beneath the layers of platinum surface in order to mimic the constant temperature heat bath. As the potential function between water and platinum surface, two different models developed by Spohr & Heinzinger [8] and Zhu & Philpott [9] were employed. These potential models were derived from the extended Hückel calculations between a water molecule and a platinum cluster. As the initial condition, crystal water with the density of liquid water at 350 K was placed on the center of the platinum surface. For the initial 100 ps, velocity scaling was used for the temperature control. After this initial rough control, only the phantom heat bath was used as the temperature control at 350K. During the velocity scaling temperature control in 100 ps, the liquid vapor interface was already in semi-spherical shape. Then, the gradual spreading of the water droplet was observed. The area of contact region between water and platinum was monitored to examine the equilibrium condition. After long enough time, the
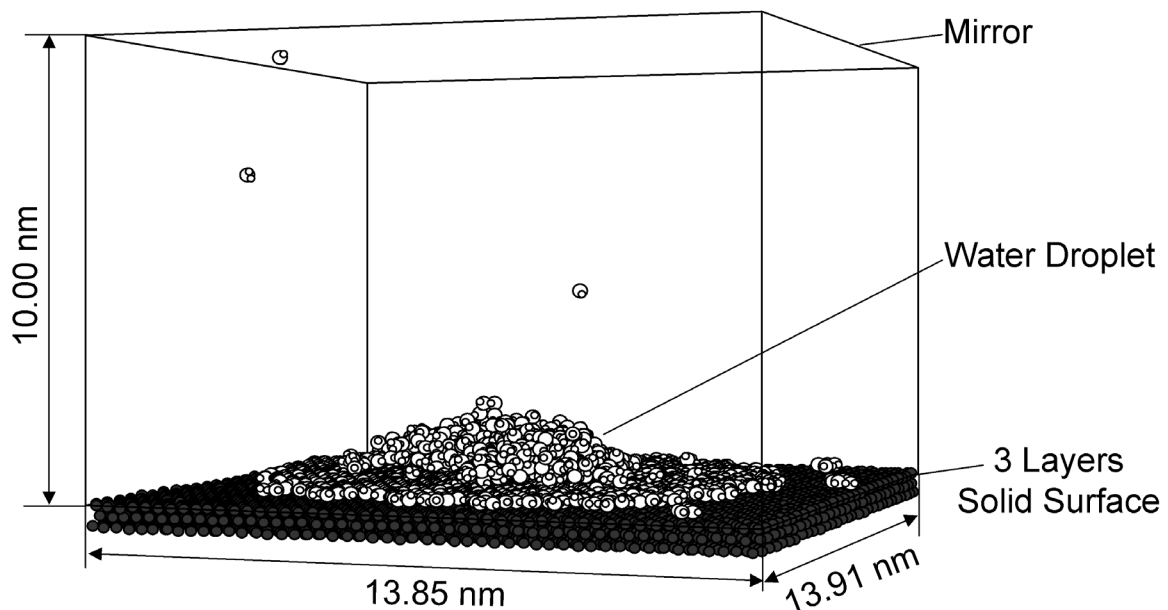

Fig. 1 A snapshot of equilibrium structure of water on Pt (111) surface at 350 K with Z-P potential. A droplet shape was observed on a monolayer water film.
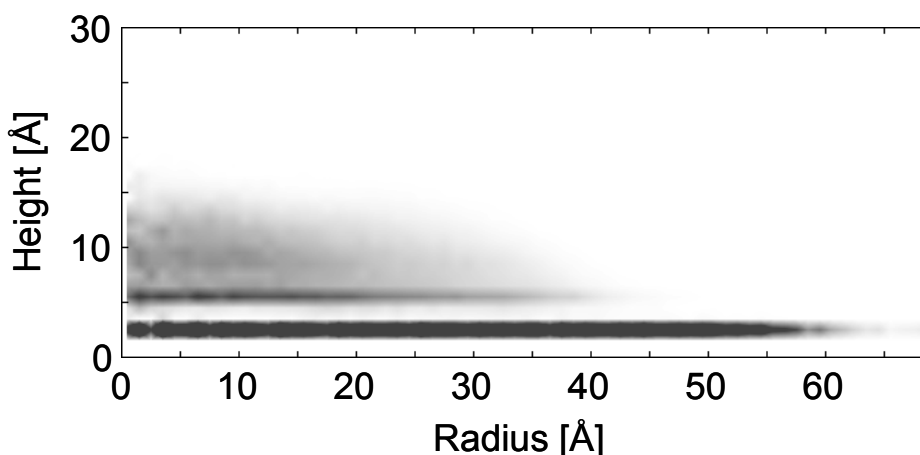
Fig. 2 Two-Dimensional density distribution of an equilibrium droplet as in Fig. 1. By disregarding the monolayer water, the contact angle can be measured as approximately 20°.

equilibrium structure was observed. The droplet finally spread to simply monolayer film for S-H potential on the fcc (111) surface. On the other hand, in the case of Z-P potential, a stable liquid droplet with a certain contact angle on the monolayer water was observed as in Fig. 1 and Fig. 2. This is the first realization of stable droplet structure on the precursor film with molecular dynamics level calculation. The existence of the contact angle of liquid water on a monolayer water can be explained that because monolayer water molecules are so densely allocated on Pt surface, then, the binding energy between monolayer water and droplet water are reduced.

Furthermore, the contact phenomena was drastically dependent on the surface structure of Pt. The dependence of contact angle on three examined surface orientations (111), (100) and (110) were explained by the previous idea that less wetting monolayer was realized by the higher density of water molecules.

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